checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: shelx

```
Bond precision:   Pb- O = 0.0036 A         Wavelength=0.71075

Cell:             a=9.1765(18)     b=12.340(3)         c=5.0092(10)
                  alpha=90         beta=101.01(3)      gamma=90
Temperature:      100 K

                 Calculated                  Reported
Volume           556.8(2)                    556.8(2)
Space group      P 21/m                      P 21/m
Hall group       -P 2yb                      -P 2yb
Moiety formula   Fe2 H3 Mn2 O15 P3 Pb        ?
Sum formula      Fe2 H3 Mn2 O15 P3 Pb        FeM2 H3 Mn2 O15 P3 Pb
Mr               764.71                      763.70
Dx,g cm-3        4.561                       4.555
Z                2                           2
Mu (mm-1)        20.345                      20.344
F000             704.0                       702.0
F000'            701.21
h,k,lmax         12,16,6                     12,16,6
Nref             1501                        1417
Tmin,Tmax        0.672,0.903                 0.342,0.435
Tmin'            0.659

Correction method= # Reported T Limits: Tmin=0.342 Tmax=0.435
AbsCorr = MULTI-SCAN

Data completeness= 0.944            Theta(max)= 28.700

R(reflections)= 0.0207( 1417)                wR2(reflections)=
                                             0.0723( 1417)
S = 0.927                  Npar= 119
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level A

```
PLAT184_ALERT_1_A Missing _cell_measurement_theta_min Value ......     Please Do !
```

Author Response: The cell measurement theta min Value was not recorded.

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PLAT185_ALERT_1_A Missing _cell_measurement_theta_max Value ......     Please Do !
```

Author Response: The cell measurement theta max Value was not recorded.

Alert level B

```
ABSMU01_ALERT_1_B  The ratio of given/expected absorption coefficient lies
               outside the range 0.95 <> 1.05
            Calculated value of mu =    19.091
            Value of mu given      =    20.344
CHEMW01_ALERT_1_B  The ratio of given/expected molecular weight as calculated
            from the _chemical_formula_sum lies outside
            the range 0.95 <> 1.05
            Calculated formula weight =   708.8590
            Formula weight given      =   763.7000
PLAT005_ALERT_5_B No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT029_ALERT_3_B _diffrn_measured_fraction_theta_full value Low .      0.954 Why?
PLAT420_ALERT_2_B D-H Bond Without Acceptor  Oh8      --H8       .     Please Check
PLAT964_ALERT_2_B SHELXL WEIGHT Par. Values in CIF & RES Differ ..     Please Check
```

Alert level C

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ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
            a literature citation. This should be contained in the
            _exptl_absorpt_process_details field.
            Absorption correction given as multi-scan
RADNW01_ALERT_1_C  The radiation wavelength lies outside the expected range
            for the supplied radiation type. Expected range 0.71065-0.71075
            Wavelength given =    0.71075
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..       1.01 Check
PLAT213_ALERT_2_C Atom O2              has ADP max/min Ratio .....        3.1 oblate
PLAT711_ALERT_1_C BOND    Unknown or Inconsistent Label ..........         Pb Check
                    PB          O4
PLAT711_ALERT_1_C BOND    Unknown or Inconsistent Label ..........         Pb Check
                    PB          O4
PLAT711_ALERT_1_C BOND    Unknown or Inconsistent Label ..........         Pb Check
                    PB          O2
PLAT711_ALERT_1_C BOND    Unknown or Inconsistent Label ..........         Pb Check
                    PB          OH8
PLAT711_ALERT_1_C BOND    Unknown or Inconsistent Label ..........         Pb Check
                    PB          O5
PLAT711_ALERT_1_C BOND    Unknown or Inconsistent Label ..........         Pb Check
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                    PB          O5
PLAT711_ALERT_1_C BOND    Unknown or Inconsistent Label ..........         Pb Check
                    PB          O6
PLAT711_ALERT_1_C BOND    Unknown or Inconsistent Label ..........         Pb Check
                    PB          O6
PLAT711_ALERT_1_C BOND    Unknown or Inconsistent Label ..........         Pb Check
                    PB          O7
PLAT711_ALERT_1_C BOND    Unknown or Inconsistent Label ..........         Pb Check
                    PB          O7
```

Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
            _chemical_formula_sum and the formula from the _atom_site* data.
            Atom count from _chemical_formula_sum:H3 Fe1 Mn2 O15 P3 Pb1
            Atom count from the _atom_site data:  H3 Fe2 Mn2 O15 P3 Pb1
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
            symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z    2
           From the CIF: _chemical_formula_sum  FeM2 H3 Mn2 O15 P3 Pb
           TEST: Compare cell contents of formula and atom_site data
           WARNING: Unexpected atom type is in site list: Fe
           WARNING: Formula and atom_type_symbol element names mismatch.

           atom    Z*formula  cif sites diff
           FeM        4.00      0.00    4.00
           H          6.00      6.00    0.00
           Mn         4.00      4.00    0.00
           O         30.00     30.00    0.00
           P          6.00      6.00    0.00
           Pb         2.00      2.00    0.00
            WARNING: Site labels do not match formula elements
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          4 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT158_ALERT_4_G The Input Unitcell is NOT Standard/Reduced .....     Please Check
PLAT303_ALERT_2_G Full Occupancy Atom H8        with # Connections       2.00 Check
PLAT480_ALERT_4_G Long H...A H-Bond Reported H8       ..O6       .       2.73 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          5 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          2 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL     2019/3 Note
PLAT940_ALERT_3_G Fsqd Refinement With I > n * Sigma(I) Only .....     Please Check
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2 **ALERT level A** = Most likely a serious problem - resolve or explain
6 **ALERT level B** = A potentially serious problem, consider carefully
14 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
14 **ALERT level G** = General information/check it is not something unexpected

21 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

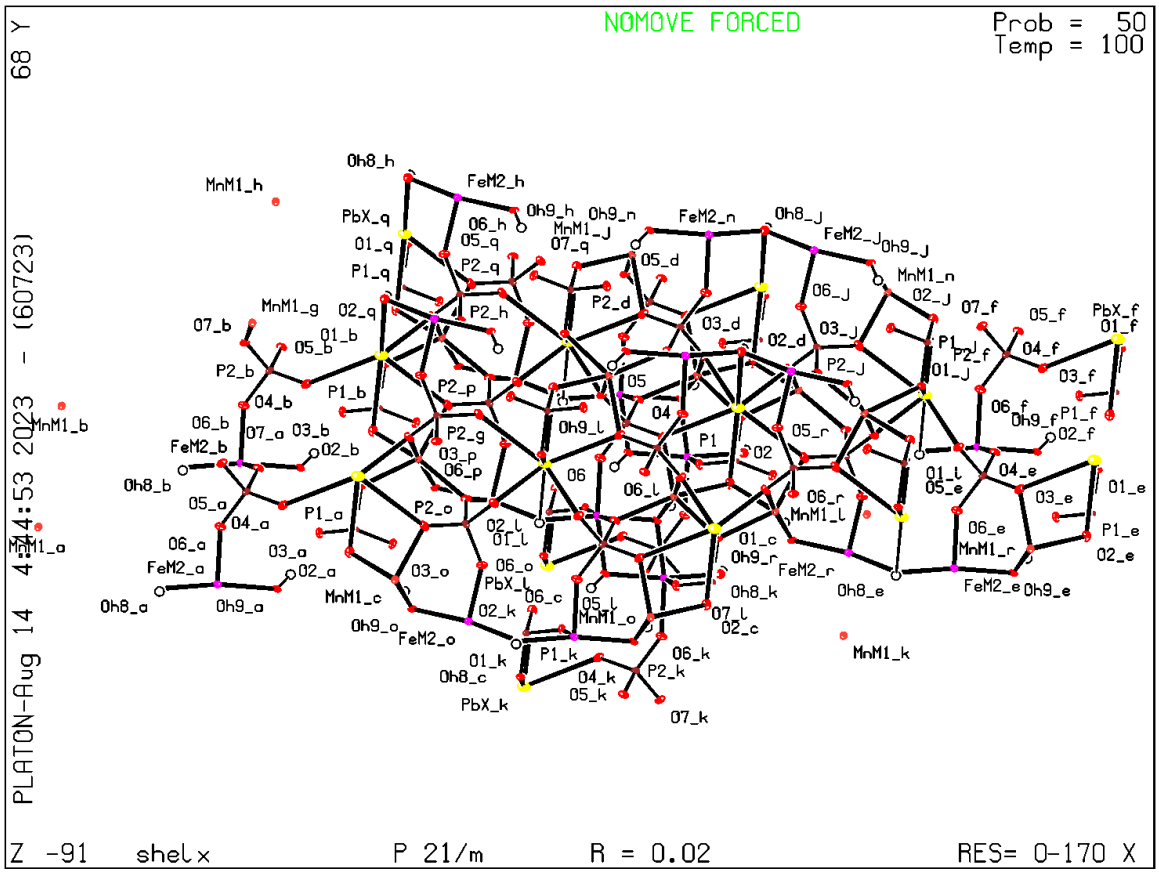
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 06/07/2023; check.def file version of 30/06/2023

Datablock shelx - ellipsoid plot